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Properties of unsaturated phospholipid bilayers: Effect of cholesterol

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Abstract

Theoretical and experimental study of the liquid crystalline phase of five different hydrated unsaturated phosphatidylcholine (PC) lipid bilayers built up by 18:0/18: 1(n-9)cis PC, 18:0/18:2(n-6)cis PC, 18:0/18:3(n-3)cis PC, 18:0/20:4(n-6)cis PC, and 18:0/22:6(n-3)cis PC molecules with 40 mol% cholesterol, and the same five pure PC bilayers have been performed at 303 K. Molecular dynamics (MD) computer simulations and self-consistent field (SCF) calculations for the study of model pure unsaturated PC and PC/cholesterol membrane systems, and the pulsed field gradient nuclear magnetic resonance (pfg NMR) technique for the study of corresponding real pure PC and PC/cholesterol membranes have been used. The lateral diffusion coefficients of the lipids in these systems, atom mass density distributions with respect to the bilayer normal, the C-H and C-C bond order parameter profiles of the lipid hydrocarbon chains have been analyzed. It has been found that mobility of PC molecules increases as the degree of their unsaturation increases (i.e., the lateral diffusion coefficients of PC molecules increase with increasing a number of double bonds in one of the lipid chains), both in pure bilayers and in bilayers with cholesterol. It has been found as well that the lateral diffusion coefficient of PC molecules of a lipid bilayer with 40 mol% cholesterol is smaller than that for the corresponding pure PC bilayer. The presence of cholesterol in a bilayer is found to promote extending of both saturated and polyunsaturated lipid chains. The effect of cholesterol on the order parameters of the double C=C bonds of polyunsaturated chains is found to be more appreciable than that for single C-C bonds of saturated chains. The theoretical (MD and SCF) results are in agreement with the results of the pfg NMR experimental study.